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Introduction to Maxwell's Equations

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This note summarizes some selected chapters of the first part of my lecture on Numerical Methods for Maxwell's Equations from last summer in Karlsruhe. It should provide some background material for the Intensive Program.

Parts of this note are extremely simple. The examples are designed to provide some insight in the numerical difficulties which are inherent in Maxwell'e equations. Most effects are demonstrated for the scalar wave equation. For more details and proofs of the results we refer to the references below.

The methods presented here cannot successfully applied to photonics; this requires far more analytical and numerical effort. Nevertheless, this note should explain why simple methods do not work.

Parts of the note are not finished. Please check our website

`http://www.mathematik.uni-karlsruhe.de/user/~wieners/MaxwellCourse.pdf`

for an updated and corrected version.

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Introduction to Maxwell's equations

Basic principles

We consider electromagnetic waves in a region $\Omega \subset \mathbb{R}^3$ with no magnetic sources, but Ω may (partly) be filled with materials that absorb electric energy.

Electro-magnetic waves are described by the following quantities:

$$\begin{array}{lll} \boldsymbol{\mathcal{E}}\colon \Omega \times [0,\infty) & \to \mathbb{R}^3 & \text{electric field intensity} \\ \boldsymbol{\mathcal{H}}\colon \Omega \times [0,\infty) & \to \mathbb{R}^3 & \text{magnetic field intensity} \\ \boldsymbol{\mathcal{D}}\colon \Omega \times [0,\infty) & \to \mathbb{R}^3 & \text{electric displacement} \\ \boldsymbol{\mathcal{B}}\colon \Omega \times [0,\infty) & \to \mathbb{R}^3 & \text{magnetic field induction} \end{array}$$

We assume that the following quantities are given:

$$\begin{array}{lll} \mathbf{J}\colon \Omega \times [0,\infty) & \to \mathbb{R}^3 & \text{electric current density} \\ \rho\colon \Omega \times [0,\infty) & \to \mathbb{R} & \text{electric charge density} \end{array}$$

We assume within this introduction that all fields are sufficiently smooth.

Physical laws

1) Faraday's Law For all (smooth and bounded) oriented two-dimensional manifolds A in Ω we have

$$\partial_t \int_A \boldsymbol{\mathcal{B}} \cdot da + \int_{\partial A} \boldsymbol{\mathcal{E}} \cdot d\ell = 0\,,$$

i.e., an electric field along the line ∂A induces a change of the magnetic introduction through the surface A.

Example Consider the square

$$A = (0,1) \times (0,1) \times \{0\}$$

with boundary

$$\partial A = (0,1) \times \{0\} \times \{0\} \cup\ \{1\} \times \{0\} \times \{0\} \cup\ (0,1) \times \{1\} \times \{0\} \cup\ \{0\} \times (0,1) \times \{0\}$$

For determining the orientation we choose the normal vector on A

$$\boldsymbol{n}(\boldsymbol{x}) \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \boldsymbol{x} \in A$$

Then, we have

$$\begin{aligned} 0 \;=\; & \partial_t \int_A \boldsymbol{\mathcal{B}} \cdot da + \int_{\partial A} \boldsymbol{\mathcal{E}} \cdot d\ell = \int_0^1 \int_0^1 \partial_t \boldsymbol{\mathcal{B}}(x_1, x_2, 0, t) \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} dx_1\, dx_2 \\ & + \int_0^1 \boldsymbol{\mathcal{E}}(x_1, 0, 0, t) \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} dx_1 + \int_0^1 \boldsymbol{\mathcal{E}}(1, x_2, 0, t) \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} dx_2 \\ & + \int_1^0 \boldsymbol{\mathcal{E}}(x_1, 1, 0, t) \cdot \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix} dx_1 + \int_1^0 \boldsymbol{\mathcal{E}}(0, x_2, t) \cdot \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix} dx_2 \end{aligned}$$

2) Ampere's Law For all $A \subset \Omega$ we have

$$\partial_t \int_A \boldsymbol{\mathcal{D}} \cdot da - \int_{\partial A} \boldsymbol{\mathcal{H}} \cdot d\ell + \int_A \boldsymbol{J} \cdot da = 0\,,$$

i.e., an electric current density $\boldsymbol{J}$ through A and a magnetic field $\boldsymbol{\mathcal{H}}$ along ∂A induces a change of the electric displacement $\boldsymbol{\mathcal{D}}$.

3) Gauß's Law for the electric field For all volumes $V \subset \Omega$ with piecewise smooth boundary we have

$$\int_{\partial V} \boldsymbol{\mathcal{D}} \cdot da - \int_V \rho\, dx = 0\,,$$

i.e. the flux of the electric displacement through ∂V coincides with the sources of the charge density in V.

4) Gauß's Law for the magnetic field For all $V \subset \Omega$ we have

$$\int_{\partial V} \boldsymbol{\mathcal{B}} \cdot da = 0\,,$$

i.e., inflow and outflow of the magnetic flux are balanced (no magnetic sources).

Definition 1. *The Maxwell p.d.e. are given by*

$$\begin{array}{rclrcl} \partial_t \boldsymbol{\mathcal{D}} - \nabla \times \boldsymbol{\mathcal{H}} & = & -\boldsymbol{J} & \partial_t \boldsymbol{\mathcal{B}} + \nabla \times \boldsymbol{\mathcal{E}} & = & 0 \\ \nabla \cdot \boldsymbol{\mathcal{D}} & = & \rho & \nabla \cdot \boldsymbol{\mathcal{B}} & = & 0 \end{array}$$

Here, we use for a vector field $\boldsymbol{u}\colon \Omega \to \mathbb{R}^3$ the notation

$$\begin{aligned} \nabla &= \begin{pmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{pmatrix} \\ \nabla \cdot \boldsymbol{u} &= \operatorname{div} \boldsymbol{u} = \partial_1 u_1 + \partial_2 u_2 + \partial_3 u_3 \\ \nabla \times \boldsymbol{u} &= \operatorname{curl} \boldsymbol{u} = \begin{pmatrix} \partial_2 u_3 - \partial_3 u_2 \\ \partial_3 u_1 - \partial_1 u_3 \\ \partial_1 u_2 - \partial_2 u_1 \end{pmatrix} \end{aligned}$$

Formally, we can derive the p.d.e. from Maxwell's equations in integral form using the theorems by Gauß and Stokes:

Gauß $\quad \displaystyle\int_V \operatorname{div} \boldsymbol{u}\, dx = \int_{\partial V} \boldsymbol{u} \cdot da$

Stokes $\quad \displaystyle\int_A \operatorname{curl} \boldsymbol{u}\, da = \int_{\partial A} \boldsymbol{u} \cdot d\ell$

Here, we use $\boldsymbol{u} \cdot da = \boldsymbol{u} \cdot \boldsymbol{n}\, da$ and $\boldsymbol{u} \cdot d\ell = \boldsymbol{u} \cdot \boldsymbol{\tau} d\ell$, the normal vector field $\boldsymbol{n}\colon A \longrightarrow \mathbb{R}^3$ and the tangential vector field $\boldsymbol{\tau}\colon \partial A \to \mathbb{R}^3$ (where the orientation of ∂A is given by $\boldsymbol{n}$).

Example (cont.) For the area $A = (0,1) \times (0,1) \times \{0\}$ we have

$$\begin{aligned}\int_A \operatorname{curl} \boldsymbol{u} \cdot da &= \int_0^1 \int_0^1 \big(\partial_1 u_2(x_1, x_2, 0) - \partial_2 u_1(x_1, x_2, 0)\big) dx_1 dx_2 \\ &= \int_0^1 \big(u_2(1, x_2, 0)\big) dx_2 - \int_0^1 \big(u_1(x_1, 1, 0) - u_1(x_1, 0, 0)\big) dx_1 = \int_{\partial A} \boldsymbol{u} \cdot d\ell\end{aligned}$$

For the volume $V = (0,1) \times (0,1) \times (0,1)$ we have

$$\begin{aligned}\int_V \operatorname{div} \boldsymbol{u} \cdot dx &= \int_0^1 \int_0^1 \int_0^1 (\partial_1 u_1 + \partial_2 u_2 + \partial_3 u_3) dx_1 dx_2 dx_3 \\ &= \int_0^1 \int_0^1 \big(\boldsymbol{u}_1(1, x_2, x_3) - u_1(0, x_2, x_3)\big) dx_2 dx_3 + \cdots = \int_{\partial V} \boldsymbol{u} \cdot \boldsymbol{n}\, da\end{aligned}$$

(general areas A and volumes V can be computed by suitable diffeomorphisms and the transformation theorem).

Thus, the theorems by Gauß and Stokes give Maxwell's equations in the form

$$\begin{aligned}&1) \quad \int_A (\partial_t \boldsymbol{\mathcal{B}} + \operatorname{curl} \boldsymbol{\mathcal{E}}) \cdot da = 0 \\ &2) \quad \int_A (\partial_t \boldsymbol{\mathcal{D}} - \operatorname{curl} \boldsymbol{\mathcal{H}} + \boldsymbol{J}) \cdot da = 0 \\ &3) \quad \int_V (\operatorname{div} \boldsymbol{\mathcal{D}} - \rho) dx = 0 \\ &4) \quad \textstyle\int_V \operatorname{div} \boldsymbol{\mathcal{B}}\, dx = 0\end{aligned}$$

for all A and V. Since A and V are arbitrary and we assume smoothness for all fields, all integrants vanish, i. e., the Maxwell p.d.e. hold for all $\boldsymbol{x} \in \Omega$.

Observation: The p.d.e. provides 8 equations for 12 unknown components of $\boldsymbol{\mathcal{B}}$, $\boldsymbol{\mathcal{E}}$, $\boldsymbol{\mathcal{D}}$, $\boldsymbol{\mathcal{H}}$. Thus, the Maxwell system has to be closed by *constitutive relations* (material laws)

$$\begin{aligned}\boldsymbol{\mathcal{D}} &= \boldsymbol{\mathcal{D}}(\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}}) \\ \boldsymbol{\mathcal{B}} &= \boldsymbol{\mathcal{B}}(\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}})\end{aligned}$$

Together, we now obtain 14 equations!

Lemma 1. *A solution of Maxwell's equations require the compatibility condition*

$$\partial_t \rho + \operatorname{div} \boldsymbol{J} = 0\,.$$

Proof. We have

$$\partial_t \int_V \rho\, dx = \partial_t \int_{\partial V} \boldsymbol{\mathcal{D}} \cdot da = \int_{\partial V} (\operatorname{curl} \boldsymbol{\mathcal{H}} - \boldsymbol{J}) \cdot da = -\int_V \operatorname{div} \boldsymbol{J}\, dx$$

since $\displaystyle\int_{\partial V} \operatorname{curl} \boldsymbol{\mathcal{H}} \cdot da = \int_V \operatorname{div}(\operatorname{curl} \boldsymbol{\mathcal{H}})\, dx = 0$ for closed surfaces. □

In our lecture, we restrict ourselves to linear constitutive laws (*linear non-dispersive materials*)

$$\begin{aligned}\boldsymbol{\mathcal{D}}(\boldsymbol{x}, t) &= \varepsilon(\boldsymbol{x})\, \boldsymbol{\mathcal{E}}(\boldsymbol{x}, t) \\ \boldsymbol{\mathcal{B}}(\boldsymbol{x}, t) &= \mu(\boldsymbol{x}) \boldsymbol{\mathcal{H}}(\boldsymbol{x}, t)\end{aligned}$$

with

$$\begin{aligned} \varepsilon\colon \Omega &\to \mathbb{R}^{3\times 3} \text{ or } \mathbb{R} && \text{electric permittivity} \\ \mu\colon \Omega &\to \mathbb{R}^{3\times 3} \text{ or } \mathbb{R} && \text{magnetic permeability} \end{aligned}$$

In general, $\varepsilon(x), \mu(x)$ are symmetric positive definite. For *isotropic materials* we have $\varepsilon(x), \mu(x) \in \mathbb{R}$.

In the special case of *homogeneous materials* we have $\varepsilon(x) \equiv \varepsilon$ and $\mu(x) \equiv \mu$ not depending on $\boldsymbol{x} \in \Omega$.

This gives Maxwell's equations for linear materials:

$$\begin{aligned} \varepsilon\partial_t\boldsymbol{\mathcal{E}} - \nabla\times\boldsymbol{\mathcal{H}} &= -\boldsymbol{J} & \qquad \mu\partial_t\boldsymbol{\mathcal{H}} + \nabla\times\boldsymbol{\mathcal{E}} &= 0 \\ \nabla\cdot(\varepsilon\boldsymbol{\mathcal{E}}) &= \rho & \nabla\cdot(\mu\boldsymbol{\mathcal{H}}) &= 0 \end{aligned}$$

Now we have 6 unknowns and 8 equations!

Lemma 2. *Assume*

$$\begin{aligned} \nabla\cdot\big(\varepsilon\boldsymbol{\mathcal{E}}(\boldsymbol{x},0)\big) &= \rho(\boldsymbol{x},0) \\ \nabla\cdot\big(\mu\boldsymbol{\mathcal{H}}(\boldsymbol{x},0)\big) &= 0 \end{aligned}$$

for the initial values at $t = 0$.

Then, we have for every solution of the p.d.e. system

$$\begin{aligned} \varepsilon\partial_t\boldsymbol{\mathcal{E}} - \nabla\times\boldsymbol{\mathcal{H}} &= -\boldsymbol{J} \\ \mu\partial_t\boldsymbol{\mathcal{H}} + \nabla\times\boldsymbol{\mathcal{E}} &= 0 \\ \partial_t\rho + \nabla\cdot\boldsymbol{J} &= 0 \end{aligned}$$

also $\nabla\cdot\big(\varepsilon\boldsymbol{\mathcal{E}}\big) = \rho$ *and* $\nabla\cdot(\mu\boldsymbol{\mathcal{H}}) = 0$ *for all* $t > 0$.

Proof. We have for $\nabla = (\partial_1, \partial_2, \partial_3)^T$ and any smooth vector field $\boldsymbol{u} = (u_1, u_2, u_3)$

$$\nabla\cdot(\nabla\times\boldsymbol{u}) = \partial_1(\partial_2 u_3 - \partial_3 u_2) + \partial_2(\partial_3 u - \partial_1 u_3) + \partial_3(\partial_1 u_2 - \partial_2 u_1) = 0\,.$$

This gives

$$\partial_t\big(\nabla\cdot(\mu\boldsymbol{\mathcal{H}})\big) = \nabla\cdot(\mu\partial_t\boldsymbol{\mathcal{H}}) = -\nabla\cdot(\nabla\times\boldsymbol{\mathcal{E}}) = 0$$

and thus $\nabla\cdot(\mu\boldsymbol{\mathcal{H}}) \equiv 0$ for all $t > 0$ as a consequence of the initial condition.
Analogously, we obtain from the compatibility equation

$$\partial_t\big(\nabla\cdot(\varepsilon\boldsymbol{\mathcal{E}}) - \rho\big) = \nabla\cdot(\nabla\times\boldsymbol{\mathcal{H}} - \boldsymbol{J}) - \partial_t\rho = \nabla\cdot(\nabla\times\boldsymbol{\mathcal{H}}) = 0$$

which finally proves $\nabla\cdot\big(\varepsilon\boldsymbol{\mathcal{E}}\big) = \rho$. □

A further constitutive law is Ohm's Law $\boldsymbol{J} = \sigma\boldsymbol{\mathcal{E}} + \boldsymbol{J}_a$ for given

$$\begin{aligned} \sigma\colon \Omega &\to \mathbb{R}, \quad \sigma(x) > 0 && \text{conductivity} \\ \boldsymbol{J}_a\colon \Omega &\to \mathbb{R}^3 && \text{applied current density} \end{aligned}$$

A special case are electro-magnetic waves in the vacuum: there, we have

$$\rho \equiv 0; \qquad \boldsymbol{J} \equiv 0, \qquad \sigma \equiv 0, \qquad \varepsilon \equiv \varepsilon_0, \qquad \mu \equiv \mu_0\,.$$

We choose physical units such that $\varepsilon_0 = \mu_0 = 1$.

A special case for Maxwell's equations: the wave equation

Lemma 3. *Consider a homogeneous and isotropic material (i.e., the parameters $\varepsilon, \mu, \sigma \in \mathbb{R}$ are constant) without charges (i.e., $\rho \equiv 0$) and without applied currents ($\boldsymbol{J}_a \equiv 0$), i.e.,*

$$\begin{aligned} \varepsilon \partial_t \boldsymbol{\mathcal{E}} - \nabla \times \boldsymbol{\mathcal{H}} &= -\sigma \boldsymbol{\mathcal{E}} \qquad & \mu \partial_t \boldsymbol{\mathcal{H}} + \nabla \times \boldsymbol{\mathcal{E}} &= 0 \\ \nabla \cdot (\varepsilon \boldsymbol{\mathcal{E}}) &= 0 \qquad & \nabla \cdot (\mu \boldsymbol{\mathcal{H}}) &= 0. \end{aligned}$$

Then we have

$$\begin{aligned} &\partial_t^2 \boldsymbol{\mathcal{E}} - c^2 \Delta \boldsymbol{\mathcal{E}} + \frac{\sigma}{\varepsilon} \partial_t \boldsymbol{\mathcal{E}} = 0 \\ &\partial_t^2 \boldsymbol{\mathcal{H}} - c^2 \Delta \boldsymbol{\mathcal{H}} + \frac{\sigma}{\mu} \partial_t \boldsymbol{\mathcal{H}} = 0 \end{aligned}$$

where $c = \frac{1}{\sqrt{\varepsilon\mu}}$ is the wave velocity and $\Delta = \partial_1^2 + \partial_2^2 + \partial_3^2$ is the Laplacian.

Observation: We obtain 6 decoupled (damped) scalar wave equations with coupling via the initial conditions

$$\begin{aligned} &\boldsymbol{\mathcal{E}}(x,0) = \boldsymbol{\mathcal{E}}_0(x)\,, \qquad \boldsymbol{\mathcal{H}}(x,0) = \boldsymbol{\mathcal{H}}_0(x)\,, \\ &\partial_t \boldsymbol{\mathcal{H}}(x,0) = -\frac{1}{\mu} \nabla \times \boldsymbol{\mathcal{E}}_0(x)\,, \qquad \partial_t \boldsymbol{\mathcal{E}}(x,0) = \frac{1}{\varepsilon} \nabla \times \boldsymbol{\mathcal{H}}_0(x) - \frac{\sigma}{\varepsilon} \boldsymbol{\mathcal{E}}_0(x) \end{aligned}$$

Proof. We have for a vector field $\boldsymbol{u} \colon \Omega \to \mathbb{R}^3$

$$\begin{aligned} \nabla \times \nabla \times \boldsymbol{u} &= \begin{pmatrix} \partial_2(\partial_1 u_2 - \partial_2 u_1) - \partial_3(\partial_3 u_1 - \partial_1 u_3) \\ \partial_3(\partial_2 u_3 - \partial_3 u_2) - \partial_1(\partial_1 u_2 - \partial_2 u_1) \\ \partial_1(\partial_3 u_1 - \partial_1 u_3) - \partial_2(\partial_2 u_3 - \partial_2 u_3) \end{pmatrix} + \begin{pmatrix} \partial_1^2 u_1 - \partial_1^2 u_1 \\ \partial_2^2 u_2 - \partial_2^2 u_2 \\ \partial_3^2 u_3 - \partial_3^2 u_3 \end{pmatrix} \\ &= \begin{pmatrix} \partial_1 \operatorname{div} \boldsymbol{u} - \Delta u_1 \\ \partial_2 \operatorname{div} \boldsymbol{u} - \Delta u_2 \\ \partial_3 \operatorname{div} \boldsymbol{u} - \Delta u_3 \end{pmatrix} = \nabla(\nabla \cdot \boldsymbol{u}) - \Delta \boldsymbol{u} \end{aligned}$$

This gives

$$\begin{aligned} \mu\varepsilon \partial_t^2 \boldsymbol{\mathcal{E}} &= \mu \partial_t (\nabla \times \boldsymbol{\mathcal{H}} - \sigma \boldsymbol{\mathcal{E}}) \\ &= \nabla \times (\mu \partial_t \boldsymbol{\mathcal{H}}) - \mu\sigma \partial_t \boldsymbol{\mathcal{E}} \\ &= -\nabla \times \nabla \times \boldsymbol{\mathcal{E}} - \mu\sigma \partial_t \boldsymbol{\mathcal{E}} \\ &= -\nabla\big(\varepsilon^{-1} \underbrace{\nabla \cdot (\varepsilon \boldsymbol{\mathcal{E}})}_{=0}\big) + \Delta \boldsymbol{\mathcal{E}} - \mu\sigma \partial_t \boldsymbol{\mathcal{E}}\,. \end{aligned}$$

The rest follows analogously. □

Remark 4. *This result is restricted to smooth solution in homogeneous media, i.e., we obtain only solutions for special cases!*

Harmonic plane waves Consider a scalar function $u\colon \mathbb{R}^3 \to \mathbb{C}$ with

$$Lu := \partial_t^2 u - c^2 \Delta u + \sigma \partial_t u = 0$$

Make the ansatz $u(\boldsymbol{x},t) = \exp\big(\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})\big)$ with *wave number* $\boldsymbol{k} \in \mathbb{R}^3$ and frequency ω. We have

$$\begin{aligned} \partial_t \exp\big(\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})\big) &= \mathrm{i}\omega \exp\big(\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})\big) \\ \partial_j \exp\big(\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})\big) &= -\mathrm{i}k_j \exp\big(\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})\big) \end{aligned}$$

This gives the *dispersion relation*

$$Lu = 0 \iff -\omega^2 + c|\boldsymbol{k}|^2 + \sigma \mathrm{i}\omega = 0$$

Observation: Without damping (i.e., $\sigma = 0$) we have $\omega(\boldsymbol{k}) = c|\boldsymbol{k}|$ and $c = \frac{\omega(\boldsymbol{k})}{|\boldsymbol{k}|}$.
We call a medium *non-dispersive* if the velocity of waves in the medium is not depending on the frequency ω. In fact, only the vacuum is non-dispersive, but in many cases the non-dispersive effect are neglected.

Solutions of the wave equation in 1-d We consider $\Omega \subset \mathbb{R}$ and $u\colon \Omega \to \mathbb{C}$ with $\partial_t^2 u = c^2 \partial_x^2 u$.

A) Travelling waves $u(x,t) = F(x \pm ct)$ on $\Omega = \mathbb{R}$ for a given function $F\colon \mathbb{R} \to \mathbb{R}$

$$\Longrightarrow \partial_t^2\, F(x \pm ct) = c^2\, F''(x \pm ct) = c^2 \partial_x^2\, F(x \pm ct)$$

B) Harmonic waves $u(x,t) = \exp\big(\mathrm{i}(\omega t - kx)\big)$ on $\Omega = \mathbb{R}$ for $\frac{\omega}{k} = c$. We have

wave length λ	wave number $k = \frac{2\pi}{\lambda}$
frequency f	angular frequency $\omega = 2\pi f$.

C) The Cauchy problem for $\Omega = \mathbb{R}$

$$\partial_t^2 u = c^2 \partial_x u \qquad u(x,0) = u_0(x) \qquad \partial_t u(x,0) = v_0(x)$$

is explicitly solved by

$$u(x,t) = \frac{1}{2}\big(u_0(x-ct) + u_0(x+ct)\big) + \frac{1}{c}\int_{x-ct}^{x+ct} v_0(y)dy$$

Example: $u_0 \equiv 0,\ v_0(x) = \delta_0(x)$ (Delta distribution) gives

$$u(x,t) = \begin{cases} 1 & -ct \le x \le ct \\ 0 & \text{else} \end{cases}$$

D) For the Cauchy problem for $\Omega = (0,\pi)$ with homogeneous boundary conditions $u(0,t) = u(\pi,t) = 0$ for $t > 0$ we make the ansatz

$$u(x,t) = \sum_{n=1}^{\infty} \hat{u}_n(t)\sin(nx)$$

This gives

$$\sum_{n=1}^{\infty} \hat{u}_n''(t)\sin(nx) = -c^2 \sum_{n=1}^{\infty} n^2 \hat{u}_n(t)\sin(nx)\,,$$

i.e., $\hat{u}_n'' + c^2 n^2 \hat{u}_n = 0$ for $t > 0$. The Fourier representation of the initial values

$$u_0(x) = \sum_{n=1}^{\infty} a_n \sin(nx) \quad v_0(x) = \sum_{n=1}^{\infty} b_n \sin(nx)$$

give $\hat{u}_n(0) = a_n$ and $\hat{u}_n'(0) = b_n$. Then we have

$$\hat{u}_n(t) = a_n \cos(cnt) + \frac{1}{nc} b_n \sin(cnt)$$

Problem 1 Find (analytically) the Fourier representation of the solution of the scalar wave equation for the initial values $u_0 \equiv 1$ and $v_0 \equiv 0$. (Note that these initial values are not compatible with the boundary conditions for $t > 0$.)

Solution of Problem 1 We have

$$a_n = \frac{2}{\pi}\int_0^{\pi} \sin(nx)dx = \begin{cases} \frac{4}{n\pi} & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$

and $b_n \equiv 0$. This gives

$$\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} a_n \cos(cnt)\sin(nx) \\ &= \tfrac{1}{2}\sum_{n=1}^{\infty} a_n \Big(\sin(nx+nct) + \sin(nx-nct)\Big) \\ &= \tfrac{1}{2}\big(u_0(x+ct) + u_0(x-ct)\big) \end{aligned}$$

with the periodic extension of u_0

$$u_0(x) = \begin{cases} 1 & x \in (0,\pi) + 2\pi\mathbb{Z} \\ 0 & x \in \pi\mathbb{Z} \\ -1 & x \in (-\pi,0) + 2\pi\mathbb{Z} \end{cases}$$

1 Explicit numerical schemes for of the scalar wave equation

Let the wave velocity $c > 0$ be constant. Consider the second order initial value problem

$$\begin{aligned} &\partial_t^2 u(x,t) = c^2 \partial_x^2 u(x,t)\,, \qquad (x,t) \in \mathbb{R} \times \mathbb{R} \\ &u(x,0) = u_0(x)\,, \qquad \partial_t u(x,0) = v_0(x)\,, \qquad x \in \mathbb{R} \end{aligned}$$

and an approximation $(u_j^n)_{n,j} \in \mathbb{Z} \times \mathbb{Z}$ on the regular grid $(\Delta x)\mathbb{Z} \times (\Delta t)\mathbb{Z} \subset \mathbb{R} \times \mathbb{R}$, where

$\Delta x > 0$	spatial mesh size,	$x_j = j\Delta x$
$\Delta t > 0$	time step size,	$t_n = n\Delta t$

Problem 2 Let $g \in C^4(\mathbb{R})$ and $h > 0$. Prove

$$\left|g''(x) - \frac{1}{h^2}\big(g(x-h) - 2g(x) + g(x+h)\big)\right| \le \frac{h^2}{12} \max_{\xi \in [x-h,x+h]} \left|g''''(\xi)\right|.$$

Solution of Problem 2 We have the Taylor expansion

$$g(x+h) = g(x) + hg'(x) + \frac{1}{2}h^2 g''(x) + \frac{1}{6}h^3 g'''(x) + \frac{1}{24}h^4 g''''(\xi_1)$$

$$g(x-h) = g(x) - hg'(x) + \frac{1}{2}h^2 g''(x) - \frac{1}{6}h^3 g'''(x) + \frac{1}{24}h^4 g''''(\xi_2)$$

with $\xi_1 \in [x, x+h]$, $\xi_2 \in [x-h, x]$. This gives

$$g(x+h) + g(x-h) - 2g(x) = h^2 g''(x) + \frac{1}{24}h^4\big(g''''(\xi_1) + g''''(\xi_2)\big)\,.$$

This motivates the following *finite difference scheme*: Define the initial values

$$\begin{aligned} &u_j^0 = u_0(x_j) && j \in \mathbb{Z} \\ &u_j^1 = u_j^0 + \Delta t\, v_0(x_j) && j \in \mathbb{Z} \end{aligned}$$

and then, for $n = 1, 2, ...$ compute

$$\frac{1}{(\Delta t)^2}\big(u_j^{n+1} - 2u_j^n + u_j^{n-1}\big) = c^2 \frac{1}{(\Delta x)^2}\big(u_{j+1}^n - 2u_j^n + u_{j-1}^n\big) \qquad j \in \mathbb{Z} \qquad n = 2, 3, \ldots$$

Problem 3 We consider the special case $\Delta t = \frac{\Delta x}{c}$ (the *magic time step*).
Show that for the magic time step a travelling wave $u(x,t) = F(x \pm ct)$ with consistent initial values

$$u_j^0 = F(j\Delta x),\ u_j^1 = F(j\Delta x \pm c\Delta t) = F\big((j \pm 1)\Delta x\big)$$

is exactly preserved.
Show that the harmonic wave $u(x,t) = \exp\big(\mathrm{i}(\omega t - kx)\big)$ with $\omega/k = \pm c$ has the same property.

Solution of Problem 3 For the magic time step $\Delta t = \frac{\Delta x}{c}$ we have

$$u_j^{n+1} - 2u_j^n + u_j^{n-1} = u_{j+1}^n - 2u_j^n + u_{j-1}^n \tag{1}$$

A) Consider a travelling wave $u(x,t) = F(x \pm ct)$ with consistent initial values

$$u_j^0 = F(j\Delta x),\ u_j^1 = F(j\Delta x \pm c\Delta t) = F\big((j \pm 1)\Delta x\big)$$

Inserting (1) gives for $n > 1$ (by induction)

$$\begin{aligned} u_j^{n+1} &= u_{j+1}^n + u_{j-1}^n - u_j^{n-1} \\ &= F\big((j+1)\Delta x \pm cn\Delta t\big) + F\big((j-1)\Delta x \pm cn\Delta t\big) - F\big(j\Delta x \pm c(n-1)\Delta t\big) \\ &= F\Big(\big(j \pm (n+1)\big)\Delta x\Big)\,. \end{aligned} \tag{2}$$

Thus, the travelling wave is exactly preserved for the magic time step.

B) The harmonic wave $u(x,t) = \exp\big(\mathrm{i}(\omega t - kx)\big) = F(x \pm ct)$ is a travelling wave with $F(x) = \exp(-\mathrm{i}kx)$, since $|\omega/k| = c$.

Program 1 Write a test program for the scalar wave equation in the interval $[0,a]$ with periodic boundary conditions. Choose $J > 1$ and set $\Delta x = a/J$. Choose the magic time step $\Delta t = \Delta x/c$. For given $u_0^0, u_1^0, ..., u_{J-1}^0, u_J^0 = x_0$ and $v_0^0, v_1^0, ..., v_{J-1}^0, v_J^0 = v_0^0$ set

$$u_j^1 = u_j^0 + \Delta t\, v_j^0\,,$$

and then compute u_j^n for $j = 0, ..., J$ and $n = 2, ..., N$ using the finite difference scheme (2).
Use the parameters $f = 1$, $\omega = 2 * \pi * f$, $k = 2 * \pi$, $c = \omega/k = 1/f$, $\lambda = c/f$ and $a = 3\lambda$.
Start with consistent initial values for the harmonic wave $u(x,t) = \sin(\omega t - kx)$.
Show that the method works fine if $N \ll J$.
Why does the method fail for large N?

Solution of Program 1 We provide a short script in *octave* (Matlab-similar syntax). Unfortunately, indexing starts with 1.

```
J = 500;
N = 20;

pi = 4 * atan(1);
f = 1;
omega = 2 * pi * f;
k = 2 * pi;
c = omega / k;
lambda = c / f;

a = 3 * lambda;
dx = a / J;
dt = dx / c;

x = [0:dx:a];
axis("manual",[0,a,-2,2])
```

```
t = 0;
u0 = sin(omega*t-k*x);
v0 = omega * cos(omega*t-k*x);

u = sin(omega*t-k*x);
plot(x,[u;u0]);

t = dt;
u1 = u0 + dt * v0;

u = sin(omega*t-k*x);
plot(x,[u;u1]);

for n=1:N
    t = t + dt;
    u = sin(omega*t-k*x);
    for j=2:J
        u2(j) = u1(j+1) + u(j-1) - u0(j);
    end;
    u2(1) = u1(2) + u(J) - u0(1);
    u2(J+1) = u2(1);
    plot(x,[u;u2]);
    u0 = u1;
    u1 = u2;
end;
```

For $N \geq 70$ oscillations start due to rounding errors, which leads to a complete failure for larger N.

Numerical dispersion

Consider a harmonic wave $u(x,t) = \exp\big(\mathrm{i}(\omega t - kx)\big)$. The equation $\partial_t^2 u = c^2 \partial_x^2 u$ gives the dispersion relation $\omega^2 = c^2 k^2$ (the *dispersion* defines a relation of k and $\omega(k)$), and we define

$$\begin{array}{lll} \text{phase velocity} & v_p = \frac{\omega(k)}{k} & (= \pm c) \\ \text{group velocity} & v_g = \frac{d\omega(k)}{dk} & (= \pm c) \end{array}$$

Note that we have $\frac{d}{dk}\omega^2 = 2\omega\frac{d\omega}{dk} = 2c^2 k$, which gives $v_p v_g = c^2$.
In particular we observe, since the harmonic wave has no dispersion, that $|v_p| = |v_g| = c$.

Now we study phase velocity and group velocity for numerical approximations of the harmonic wave. The ansatz $u_j^n = \exp\big(\mathrm{i}(\omega n\Delta t - \tilde{k} j\Delta x)\big)$ with some $\tilde{k}$ in the finite difference scheme

$$u_j^{n+1} = \Big(\frac{c\Delta t}{\Delta x}\Big)^2 (u_{j+1}^n - 2u_j^n + u_{j-1}^n) + 2u_j^n - u_j^{n-1} \tag{3}$$

yields

$$\begin{aligned} \exp\big(\mathrm{i}(\omega(n+1)\Delta t - \tilde{k} j\Delta x)\big) &= \big(\tfrac{c\Delta t}{\Delta x}\big)^2 \exp\big(\mathrm{i}(\omega n\Delta t - \tilde{k} j\Delta x)\big)\ \big(\exp(-\mathrm{i}\tilde{k}\Delta x) - 2 + \exp(\mathrm{i}\tilde{k}\Delta x)\big) \\ &\quad + 2\exp\big(\mathrm{i}(\omega n\Delta t - \tilde{k} j\Delta x)\big) - \exp\big(\mathrm{i}(\omega(n-1)\Delta t - \tilde{k} j\Delta x)\big) \end{aligned}$$

which gives the *numerical dispersion relation*

$$\cos(\omega\Delta t) - 1 = \big(\frac{c\Delta t}{\Delta x}\big)^2\big(\cos(\tilde{k}\Delta x) - 1\big)\,.$$

For the magic time step $\Delta t = \frac{\Delta x}{c}$ we obtain $\tilde{k} = k$. In case of $\Delta t \neq \frac{\Delta x}{c}$ we obtain *numerical dispersion*: Consider $\Delta x = ac\Delta t$ and $\Delta t \to 0$

$$\begin{aligned}
&\implies\ 1 - \tfrac{1}{2}(\omega\Delta t)^2 + O(\Delta t^4) - 1 = \tfrac{1}{a^2}\Big(1 - \tfrac{1}{2}\big(\tilde{k}ac\Delta t\big)^2 + O(\Delta x^4) - 1\Big)\\
&\implies\ \tilde{k} = \pm\tfrac{\omega}{c} + O(\Delta t^2),\ \tfrac{\omega(\tilde{k})}{\tilde{k}} = \pm c + O(\Delta t^2)
\end{aligned}$$

This gives asymptotically vanishing numerical dispersion. From

$$\begin{aligned}
&\cos\big(\omega(\tilde{k})\Delta t\big) - 1 = \big(\frac{c\Delta t}{\Delta x}\big)^2\big(\cos(\tilde{k}\Delta x) - 1\big)\\
&\underset{\frac{d}{d\tilde{k}}}{\implies}\ \frac{d\omega(\tilde{k})}{d\tilde{k}}\sin\big(\omega(\tilde{k})\Delta t\big) = c^2\frac{\Delta t}{\Delta x}\sin(\tilde{k}\Delta x)
\end{aligned}$$

we obtain for the group velocity

$$\frac{d\omega(\tilde{k})}{d\tilde{k}} = \begin{cases} \pm c & \text{for} \quad a = 1 \quad \text{(magic time step)}\\ \pm c + O(\Delta t^2) & \text{else} \end{cases}$$

Problem 4 Consider $\Delta x = \frac{\lambda}{10}$ and $\Delta t = \frac{1}{2}\frac{\Delta x}{c}$. Compute an approximation of the numerical phase velocity.

Solution of Problem 4 We have $k = \frac{2\pi}{\lambda}$ and $\omega\Delta t = kc\Delta t = k\frac{\Delta x}{2}$. The approximate solution of the equation $\cos(2\frac{2\pi}{\lambda}\Delta x) - 1 = \frac{1}{4}\,\big(\cos(\tilde{k}\Delta x) - 1\big)$ gives

$$\begin{aligned}
&\tilde{k} \approx \tfrac{0.636}{\Delta x} \qquad \big(\tfrac{\lambda}{\Delta x} = 10\big)\\
\implies\ &\tilde{v}_p = \tfrac{\omega}{\tilde{k}} \approx \tfrac{2\pi f}{0.636/\Delta x} = \tfrac{2\pi\frac{c}{\lambda}\Delta x}{0.636} \approx 0.987c \qquad \text{numerical phase velocity}
\end{aligned}$$

Stability

The harmonic wave is bounded for all times. We observe that this does not hold for the discrete scheme above, if the time step is too large.

Problem 5 Show that for all $q > 0$ the ansatz

$$u_j^n = q^n\exp(\mathrm{i}kj\Delta x)$$

is a solution of the finite difference scheme with some $\Delta t > 0$.
Show that $q \leq 1$ for $\Delta t \leq \frac{\Delta x}{c}$.

Solution of Problem 5 The ansatz gives

$$
\begin{aligned}
& \tfrac{1}{(\Delta t)^2}(q^{n+1} - 2q^n + q^{n-1}) \exp(\mathrm{i}kj\Delta x) \\
& = c^2 \tfrac{1}{(\Delta x)^2} q^n \big(\exp(\mathrm{i}k(j+1)\Delta x) - 2\exp(\mathrm{i}kj\Delta x) + \exp\big(\mathrm{i}k(j-1)\Delta x\big), \\
\implies \quad & q^2 - 2q + 1 = \tfrac{2c^2(\Delta t)^2}{(\Delta x)^2} q \big(\cos(k\Delta x) - 1 \big) \\
\implies \quad & q^2 - (2 + (\Delta t)^2 \Lambda_x) q + 1 = 0
\end{aligned}
$$

for

$$
\Lambda_x = \frac{2c^2}{(\Delta x)^2} \big(\cos(k\Delta x) - 1 \big) \in \big[\frac{-4c^2}{(\Delta x)^2}, 0 \big] \,,
$$

so that we have

$$
q = p \pm \sqrt{p^2 - 1} \text{ with } p = \frac{2 + \Lambda_x (\Delta t)^2}{2} \,.
$$

This yields $|q| \le 1$ for $p^2 - 1 \le 0$, i.e., $-1 \le p \le 1$

$$
\begin{aligned}
\implies \quad & -\tfrac{4}{(\Delta t)^2} \le \Lambda_x \le 0 \\
\implies \quad & -\tfrac{4}{(\Delta t)^2} \le -\tfrac{4c^2}{(\Delta x)^2} \iff \Delta t \le \tfrac{\Delta x}{c} \,.
\end{aligned}
$$

Consequence The magic time step is the stability bound for the numerical scheme!
The interpretation for a point source $u_0(x) = \delta_0(x)$ and $v \equiv 0$ yields:

CFL-condition (Courant-Friedrichs-Lewy 1929) Stability of a finite difference scheme requires that the domain of dependence of the continuous solution contains the numerical domain of dependence.

Program 2 Modify Program 1 for $\Delta t < \Delta x / c$ using the finite difference scheme (3).
Show that the method works for $J \approx N$.
Show that the error at a fixed time $T = N\Delta t$ is reduced by decreasing Δt (and thus increasing N).

Solution of Program 2

```
J = 50;
N = 100;
fac = 0.125;

pi = 4 * atan(1);
f = 1;
omega = 2 * pi * f;
k = 2 * pi;
c = omega / k;
lambda = c / f;
```

```
a = 3 * lambda;
dx = a / J;
dt = fac * dx / c;
q = c*c*dt*dt/(dx*dx);

x = [0:dx:a];
axis("manual",[0,a,-2,2])

t = 0;
u0 = sin(omega*t-k*x);
v0 = omega * cos(omega*t-k*x);

u = sin(omega*t-k*x);
plot(x,[u;u0]);

t = dt;
u1 = u0 + dt * v0;

u = sin(omega*t-k*x);
plot(x,[u;u1]);

for n=1:N
    t = t + dt;
    for j=2:J
        u2(j) = q * (u1(j+1)-2*u1(j)+u(j-1)) + 2*u1(j) - u0(j);
    end;
    u2(1) = q * (u1(2)-2*u1(1)+u(J)) + 2*u1(1) - u0(1);
    u2(J+1) = u2(1);

    u = sin(omega*t-k*x);
    plot(x,[u;u2]);

    u0 = u1;
    u1 = u2;
end;
```

For N = 100 and fac = 0.125 the error gets smaller.